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Chain Reactions Approach to the Initial Stages of Crude Oil Oxidation

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Abstract

© 2018 American Chemical Society. The paper focuses on the problem of the crude oil self-ignition in situ, which has not yet been solved in the general case and for a particular oilfield as well. To solve the problem of ignition, we approached from a theoretical point of view - applied the theory of chain reactions to the description of the initial stages of oxidation. The obtained dependences of heat release on time should be of a general nature for experiments in which self-ignition occurred (we called them high rate experiments) and for experiments in which fuel formation was observed (low rate experiments). We first demonstrated this relationship in the experiments we conducted by high pressure rate calorimeter (PDSC). And then we analyzed the various experiments from literature sources. The novel results of the presented approach show the probabilistic nature of the ignition and the presence of a group of processes that do not lead to ignition, in which the free radicals are not sufficiently active and the heat sink exceeds the heat release. Instead of the heat balance, a new ignition criterion - φ-factor for chain reaction, the difference in the rate of formation and death of free radicals - is derived. A positive value of φ-factor indicates the increase of energy in the system and the ignition by the chain mechanism, while a negative value indicates the attenuation of the reaction and the formation of oxidized compounds without ignition. The PDSC experiments with light crude oil oxidation were conducted under various heating rates in order to explore the ignition temperature-time dependence (the example of high rate experiments). The results show the same dependence of the process time on temperature predicted theoretically. The other types of high rate experiments (adiabatic experiments, combustion tube experiments) and low rate oxidation experiments from literature sources are also considered in terms of our approach. The comparison of different types of experiments with the obtained mathematical formulas gives a good agreement. The low rate oxidation dependences refer to the negative values of φ-factor, and high rate oxidation refers to positive φ-factor modes. Both types of experiments are in good consistency with the theoretically obtained dependence and show that the model of the chain reaction approach works well. Thus, the chain reaction approach to the ignition mechanism gives one a good consistency with experimental data and can be applied for the prediction of ignition time for air injection projects. The other result of our approach is the difference between heavy and light oil oxidation in low and high rate processes. In high rate processes, free radicals are active enough for igniting the oil, and light oils contain more free radicals of this type and are more reactive for ignition. Heavy oils have better affinity for fuel formation and oxygen addition reactions. So heavy oils can usually ignite at higher temperature than light oils.

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